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Research article

Water quality modelling under unsteady state analysis: Strategies for planning and management

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ABSTRACT

Recent water resources planning and management strategies state that the concepts of risk and variable inputs should be appraised in order to comply with multiple conditions. This becomes evident especially in environments with diverse uses of water, land use and climate change. In such a context, modelling of discharges and concentrations in rivers are valuable strategies to predict different scenarios. This research proposes an integrated analysis for modelling of flow and contaminant transport in rivers, based on hydrodynamics, time series, and water quality simulations. The first module estimates water volume and velocity, that have direct impact in pollutants transport; time series of concentrations are generated as synthetic pollutographs, using techniques based on flow conditions, time and statistical factors of a historical monitoring dataset – the objective is to match temporal scales of boundary conditions, since water quality data is usually available as irregular samples; the third module solves the advection-dispersion-reaction equation, exploring the different synthetic series as input. Results evidence that the input pollutograph, usually not explored in similar studies, may have a significant role in simulations for transport of substance in rivers under unsteady state; as consequence, corroborate with better estimates for planning strategies where temporal dynamic is relevant. The contributions lay the basis for further assessment of riverine systems linked to watershed dynamics, with multiple scenarios of data availability and input conditions.

1. Introduction

Efforts to understand and predict water quality dynamics have increased over the years. Events such as floods and droughts, contamination of drinking water and stricter laws have intensified public awareness for a proper management of this resource (Chigor et al., 2012; Ascott et al., 2016).

Rivers are the main destination of wastewater from different activities, and integrate important processes that affect environmental degradation in a watershed: atmospheric transport and deposition, surface flow, loads generations and movement, and subsurface flow in groundwater zones (Novotny, 2002). Therefore, these systems reflect the overall conditions of its surrounding environment.

Hydrodynamics simulations linked to water quality give a complete description of transport dynamics in channels, and have been recognized as an important tool in water resources management (Melching et al., 2003; Wang et al., 2013).

Modelling based on mechanistic and deterministic principles under unsteady state connect several aspects that affect pollutants distribution. Even though sophisticated techniques are available for forecasting, such as artificial intelligence, estimations based on conservation laws offer robustness and easiness to implement different system conditions (Campozano et al., 2014).

The expressions involved (mass and momentum conservation) are solved using numerical approximations, which usually require small time steps, in the order of seconds or minutes. However, contrary to hydrological data, that are often available as continuous records, water quality data usually are limited or scarce (Larentis et al., 2008; Fonseca et al., 2014).

Predictions of water quality over time are often performed with monthly data (Fonseca et al., 2014; Kanda et al., 2015) and quarterly campaigns (Larentis et al.; Chang et al., 2015). Data sampled at high frequency, on the other hand, is usually available for brief periods, which may limit the simulations also to short time prediction, such as days or a few weeks (e.g. Zuo et al., 2015; Langeveld et al., 2013).

Considering that monitoring programs have limitations

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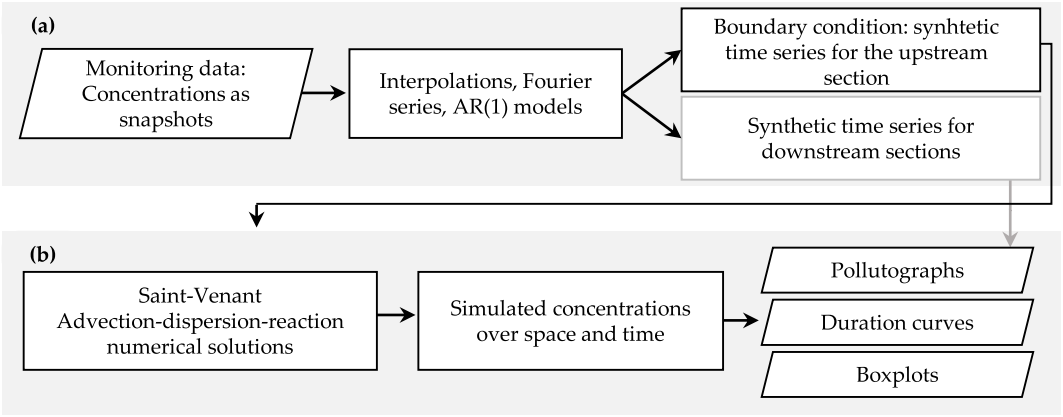

Fig. 1. Schematic of the modules in this study; (a) Synthetic pollutographs, (b) SIHQUAL: Hydrodynamic and Water Quality simulation.

Table 1
Summary of the tests performed to estimate synthetic pollutographs.

Test	Technique	Description
T1	PCHIP [(1)]	Interpolation function using monitoring discharge and concentration
T2	Fourier[(1)]	Series truncated in the fifth-term, using as parameters daily discharge and the monitored concentration
T3	AR(1)	Normal random distribution and ρ = 0.50
T4	AR(1)	Normal random distribution and ρ = 0.90
T5	Random series	Random and independent series, generated with a two parameters log-normal distribution
T6	Smoothing Spline[(1)]	Parameters: time and measured concentrations

[1] ()MATHWORKS (2017).

(uncertainties related to sample integrity and laboratory analysis, besides high costs associated with equipment and qualified people), techniques to interpolate and extrapolate the data are necessary, in order to match model requirements. In transient modelling, time series are essential as inputs and for model calibration.

Traditional monitoring plans are based on collecting samples at specific locations. This information represents snapshots at variable instants, describing specific water quality conditions. If these snapshots are not available sequentially over a longer period of time, the data may fail to capture effects of processes and parameters controlling release, fate, and transport of pollutants at other temporal scales, such as seasonal and hydrological patterns. The main challenge remains in extending this information while accounting for conditions that are continuously changing over time.

This research proposes to integrate empirical techniques (here refereed as a model that allows description of cause and effect relationships with a minimum of understanding of how the system works) to generate time series with a model for pollutant routing, using as study case the parameter Biochemical Oxygen Demand (BOD) in the Iguaçu river, located in Paraná, Brazil. The main goal is to provide a comprehensive set of evidence to encourage the integration between approaches for time series prediction, not explored in similar studies of superficial waters. This becomes an auxiliary strategy in modelling many environmental time series in high temporal resolution, integrating major aspects that may interfere in water resources planning and management decisions. At the same time, this paper provides new insights about the significance of boundary conditions in simulations for water quality under unsteady state in urban rivers.

Boundary conditions are key factors in modelling studies, since they can be one of the main sources of errors and uncertainty (Rode and Wriedt, 2006; Wang et al., 2013). Linden et al. (2015) state that, although sensitivity analysis of parameters in model outputs has been described in the literature, less often the influence of boundary conditions or input data is evaluated. Parameters usually investigated are those associated with compartment exchanges within the basin (such as export coefficients), loading inputs, and decay rates (Zhang et al., 2015; Hankin et al., 2016; Reder et al., 2017; Jia et al., 2018).

The experimental plan evaluates different approaches to define a synthetic pollutograph for the upstream section (boundary condition) using a historical dataset based on quarterly monitoring samples. The tests are based on interpolation functions, Fourier series and first order autoregressive models. Following this step, the series is propagated using the SIHQUAL model (*Simulação Hidrodinâmica e de Qualidade de Água*[1]), that solves Saint-Venant and advection-dispersion-reaction equations (Ferreira et al., 2016).

Traditionally applied in hydrological sciences, such as streamflow and rainfall forecasts (Efstratiadis et al., 2014; Pereira and Souza, 2014; Lamontagne and Stedinger, 2018), synthetic data has become a recurrent strategy in modelling water quality, providing controlled experiments that elucidate the significance of possible scenarios (e. g. McIntyre, 2004; Jia et al., 2018).

Additionally, the synthetic series are compared with steady and unsteady state modelling results, in order to verify the solutions and possible impacts in water resources management. This investigation is based on duration curves for water quality, a concept commonly suggested as a tool for planning and management (e. g. Park and Roesner, 2012; Cho and Lee, 2015).

1.1. Integrated modelling

Water quality time series have inherent characteristics, such as nonlinear trends, missing data, outliers, irregular measurement patterns, seasonal behavior, serial correlation, annual and diurnal cycles. In addition, these series are affected by intermittent events, such as rain storms (Abaurrea et al., 2011; Milne et al., 2009).

In order to match temporal scales, common strategies for data infilling or time series forecasting are: linear interpolation and regression (Adams et al., 2016), log-linear functions (Hirsch et al., 2010; Chanat et al., 2016), smoothing spline interpolations (Feng et al., 2015), Fourier series (Rodríguez et al., 2013), wavelet analysis (Dökmen and Aslan, 2013; Barzegar et al., 2017), among several others.

Time series from natural systems usually exhibit autocorrelation, a property characterized by specific functions. . In water quality, autocorrelation often is modeled with classical techniques such as autoregressive, autoregressive moving average or autoregressive integrated moving average models (e. g. Abaurrea et al., 2011; Arya and Zhang, 2015; Chen and Boccelli, 2018).

The autoregressive process of first order – AR(1) – is represented by

[1] Hydrodynamic and Water Quality Simulation.

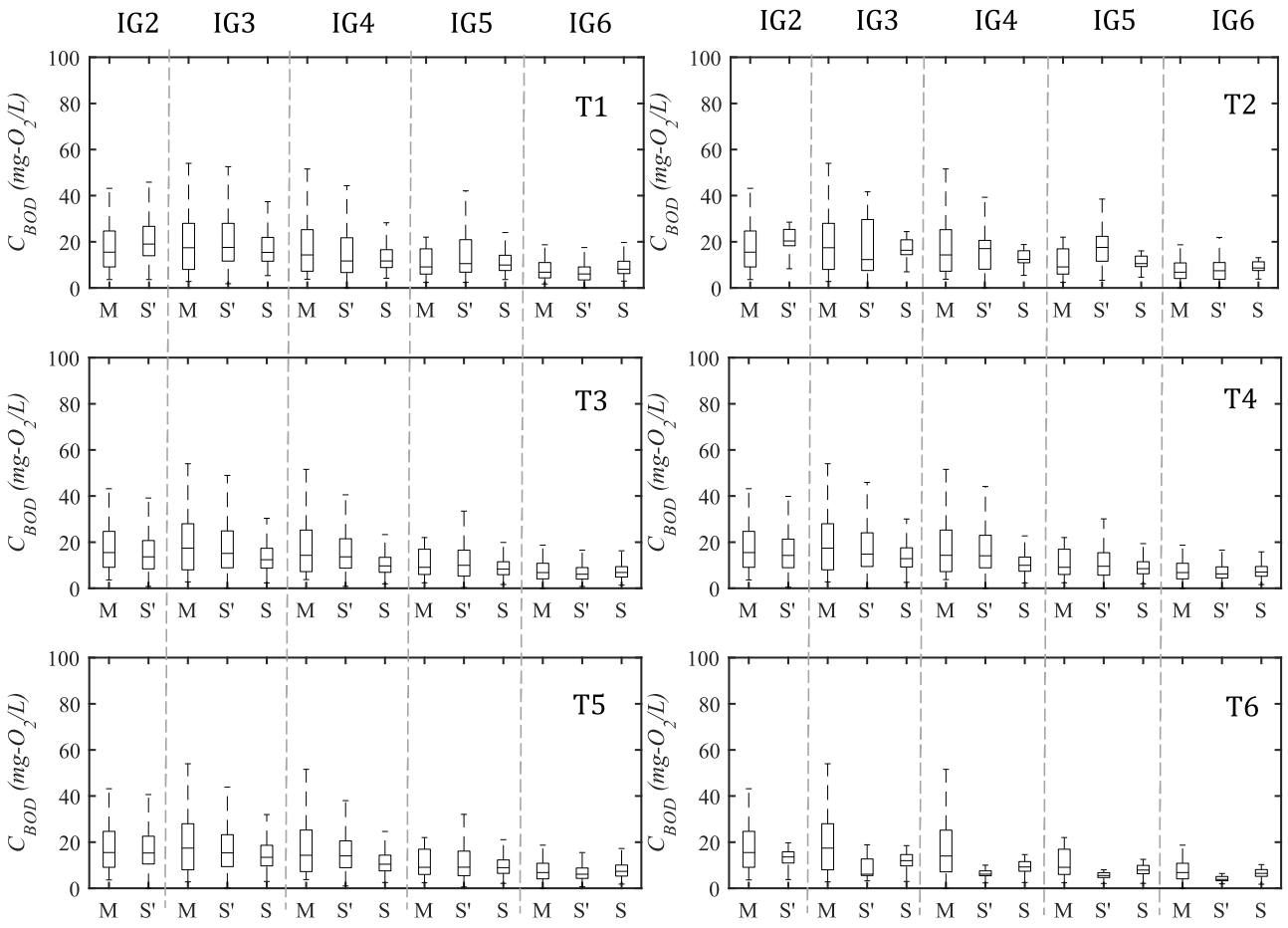

Fig. 2. Boxplots of monitoring data (M), synthetic series (*S'*) and deterministic model results (S).

a recursive equation determined by random variables, which can be written as (Loucks and Beek, 2017):

$$C_{j+1} = \mu + \rho(C_j - \mu) + z_j\sigma\sqrt{1-\rho^2} \quad (1)$$

where C is the concentration at the interval j, ρ is the sample correlation coefficient, which indicates the dependency between time intervals (deterministic component); μ is the mean of C, σ represents the standard deviation of C; z_j is the portion responsible for the random variability in the time series. The distribution of random variables is a key component in this model.

Deterministic modelling, on the other hand, accounts for transfer of matter through contours of a control volume. Several aspects are integrated, such as channel hydraulics, dispersion, transformations processes (due to chemical, biological and physical interactions), point and diffuse pollution dynamics (e. g. Kanda et al., 2015; Tang et al., 2016).

The integrated modelling approach is summarized in Fig. 1. Starting from monitoring data irregularly sampled, a first module (a) applies techniques to generate the synthetic pollutographs – interpolations, Fourier series and autoregressive model of first order, *AR(1)*. The time series of the first section is then used as boundary condition for the next module (b), while the synthetic series of other sections are used for posterior comparison with SIHQUAL outputs through graphical visualizations.

The SIHQUAL model is a one-dimensional tool to calculate discharges and concentrations over space and time in rivers. It was initially design to compare simulations under steady and unsteady state, with a module to calculate cross sections areas and velocities, and another to compute pollutants distribution (Ferreira et al., 2016).

The hydrodynamic model is based on parabolic partial difference equations for mass and momentum conservations (Saint-Venant equations), while the water quality module is conceived through the hyperbolic partial difference expression for advection-dispersion-reaction. Model details are provided in the supplementary material.

The underlying hypothesis is that the eleven years of monitoring data in the Iguaçu river adequately represent mean and standard deviation of annual concentrations. In a similar analysis, Williams et al. (2014) assumed that a sample set of five years sufficiently described sample median and log-normal standard deviation of annual concentrations; the number of samples available per year ranged between one and eight.

1.2. Synthetic pollutographs techniques

The techniques to produce synthetic pollutographs are: PCHIP (Piecewise Cubic Hermite Interpolating Polynomial) interpolation (T1), Fourier series (T2), first order autoregressive model (T3 and T4), random series (T5) and smoothing spline interpolation (T6), as described in Table 1. The supplementary material presents an additional test, with a hydrib AR(1) model that considers zero mean and unit variance, while the random component (two parameters log-normal distribution) uses the same seasonal means and standard deviation of the observed dataset.

The random component in the AR(1) models in T3 and T4 are generated with mean zero and unit variance; the parameters μ ans σ in equation (1) are the same seasonal means and standard deviation of the observed dataset (concentrations for 2005–2016). The parameter ρ is estimated, since the time series is irregular in time (therefore correlation is not specified).

Tests T1 and T2 explore the relationship between flow conditions and concentrations in channels, that can be highly variable (Zhou et al.,

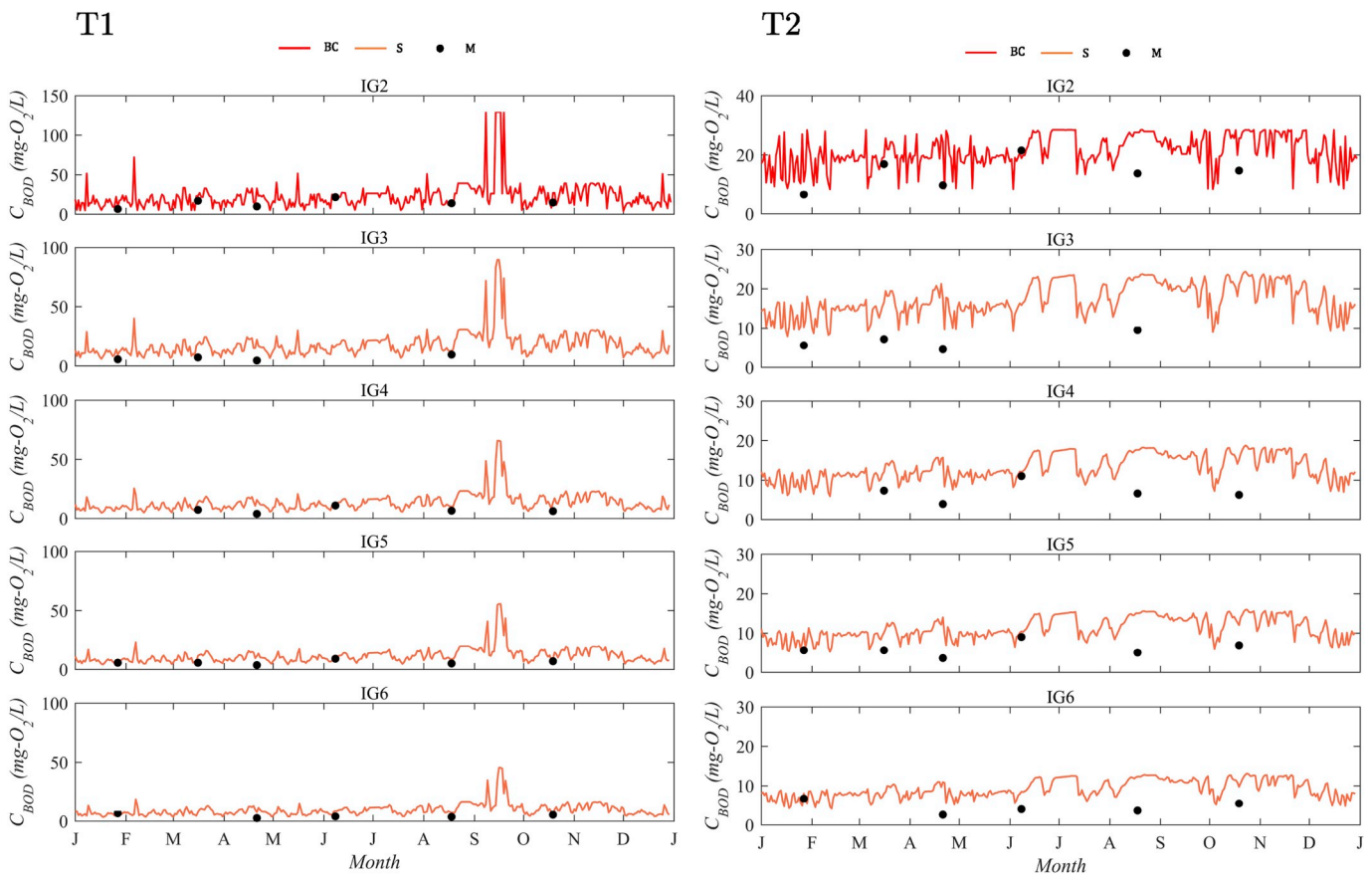

Fig. 3. Simulated daily concentrations (S) with boundary condition (BC) generated by test T1 and T2, monitoring data (M) of 2010 in each section and synthetic series (*S′*).

2011). Experiments with AR(1) aim a parsimonious analysis, compatible with the available dataset and effective to anticipate multiple scenarios. This is an advantage especially when predictions in real time are required for management strategies. Test T6, on the other hand, represents a scenario in which the input condition is similar to a steady source.

The AR(1) process assumes that the dataset has normal distribution. In order to verify this condition, quantile-quantile plots are evaluated (presented in the supplementary material), comparing quantiles of the sample data with the theoretical values from a normal distribution. The dataset indicate a violation of the normality assumption (qqplots are non-linear). Nevertheless, natural logarithms of the dataset are suitable for modelling.

2. Case study

The Upper Iguaçu watershed is located in the metropolitan area of Curitiba, capital of Paraná state (Brazil), and has approximately 2 million habitants. It covers 3000 km^2, where 30% of the state population is concentrated. A map is presented in the supplementary material. The control volume in this research is 90 km in length, draining regions with different land use: urban occupation, temporary agriculture, meadows and other vegetation categories.

The dataset selected is from 2005 to 2016, with approximately four annual campaigns. The sections of interest (IG2 – *upstream*, IG3, IG4, IG5 and IG6 – *downstream*) are located along the main channel, separated by distances between 18 and 24 km.

The parameter used as case study indicates organic matter, originated as part of biogeochemical cycles or from domestic and industrial waste. Concentrations of BOD in superficial water are used as guidelines for legal regulations in several countries, including Brazil. Data details are provided in the supplementary material.

Sections IG2, IG3 and IG4, inserted in the urban area, receive significant contributions of domestic and industrial wastes, and inputs from surface runoff. The points IG5 and IG6, on the contrary, drain an agricultural region, receiving loads from tributaries less impacted than the upstream reach.

This system remains subject of several studies (e. g. Knapik et al., 2015; Coelho et al., 2017), mostly based upon steady state analysis. Despite the advances in understanding this particular environment, these researches emphasize the need of integrating quali-quantitative aspects, in order to generate information to assist model calibration, monitoring strategies and data evaluation for sustainable and adaptable management.

To Loucks and Beek (2017), urban and agricultural development, deforestation, climatic variability, and modifications in regional management can alter the distribution of rainfall, streamflow and pollution level over time. Therefore, an analysis based upon temporal variations is required.

3. Results

Section (4.1) presents the tests in which BOD concentrations are calculated using PCHIP interpolation, Fourier series, random log-normal series, autoregressive models and fitting through smoothing spline (T1 to T6) as boundary condition.

Since data are usually sampled at infrequently intervals, and during limited events, it is not expected that models simulate daily averages equal to observed values on particular moments of the day, as mentioned by Kim et al. (2007). Therefore, following a comparison of daily simulated concentrations, boxplots and water quality duration curves are explored, in order to assess the predictive performance of the

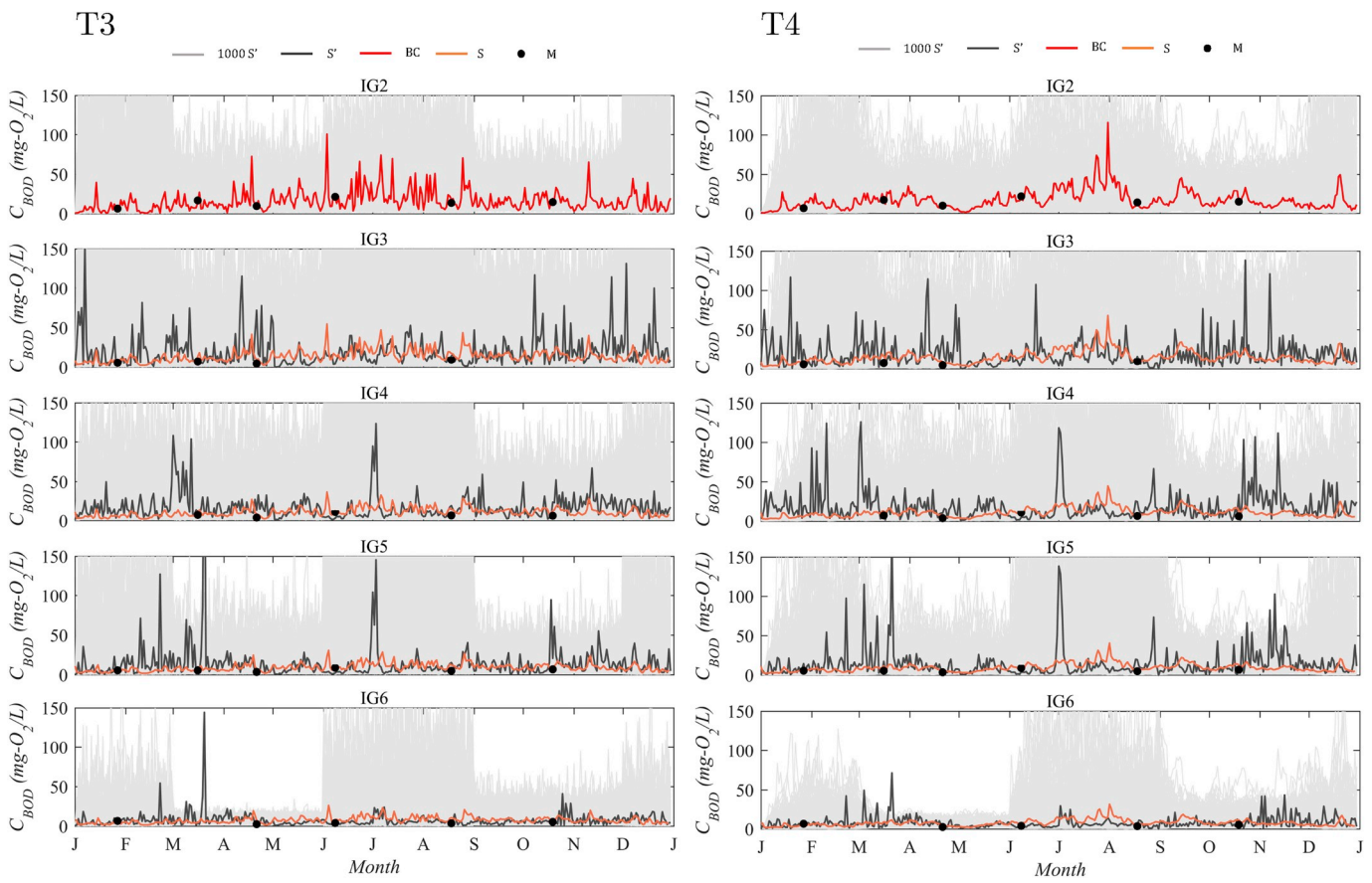

Fig. 4. Simulated daily concentrations (S) with boundary condition (BC) generated by test T3 and T4, monitoring data (M) of 2010 in each section and synthetic series (*S'*).

different approaches used in this study. Focus is on the usability of synthetic pollutographs as boundary conditions for the water quality model under unsteady state, and the effects when choosing different approaches for water resources planning and management.

3.1. Simulated time series

Because AR(1) procedures have a stochastic component (represented by the random distribution), a thousand different sets of daily concentrations are generated in tests T3, T4 and T5. A series close to the data measured in 2010 is then selected to be studied through the following procedure: (i) for each synthetic series, the concentrations corresponding to the days with monitored data in 2010 are selected; (ii) in a second step, sets are selected in which the values are between half and double of the actual data; (iii) intersecting the sets with these conditions for each point, a series is chosen out of the thousand options. In order to validate this methodology to estimate synthetic series, other case studies with different sampling frequencies are investigated (supplementary material).

Following this step, concentrations at each 50s are obtained through linear interpolation, in order to comply with the numerical solution time step. Tests T1, T2 and T6, on the other hand, directly give concentrations with this temporal resolution.

The results of each test are summarized by boxplots in Fig. 2, that compares simulated concentrations and the dataset of sampled data (boxplots *M*) – outliers are not presented. Figs. 3–5 show daily simulated means and monitoring data for the year 2010.

Concentrations in IG2 are generated applying the tests described in item 2.1, and the computed datasets of sections IG3 to IG6 are obtained when applying the SIHQUAL model for each synthetic boundary condition (boxplots *S*).

Additionally, the methods for synthetic series are applied for the following stations IG3 to IG6 (boxplots *S'*), in order to compare the series with those generated by the deterministic approach.

Synthetic series for IG2 originated with T1 and T2, presented in Fig. 3, illustrate the definition of concentrations based on discharges. September and october are periods of low flow (verified in the supplementary material, that shows hydrographs in the interval of interest); since T1 directly relates flow to concentration, in this period the model predicted high peaks of mass distribution. Test T2, on the other hand, tends to smooth concentration fluctuations in low flow periods. These behaviors are reproduced by the deterministic model in downstream sections.

For IG3 to IG6, synthetic series with T1 and T2 generated unreasonable daily mean concentrations, and are presented in the supplementary material; the boxplots, however, illustrated in Fig. 2, show interquartile values similar to the dataset. These tests indicate that predictions through PCHIP interpolation and Fourier series are not able to represent extreme values in this case.

Besides T1 and T2, tests T3, T4, and T5 generated synthetic series with interquartile and median similar to the dataset in IG3 to IG6 (although it should be stated that the series were chosen out of thousand options, and other simulations might suggest different conclusions). The Test T6 is based on interpolations using time, showing a smooth and low variation, with similar boxplots of data generated with synthetic series and deterministic modelling. This gradual variation over time unlikely is able to represent the unsteady behavior.

The boxplots for IG2 show that median concentrations and interquartile interval are more similar to the measured dataset for tests T1, T3, T4 and T5, which implies that these tests may be reliable as boundary conditions. In fact, daily average concentrations generated by these tests are close to data in the reference year, as verified in Figs. 3–5

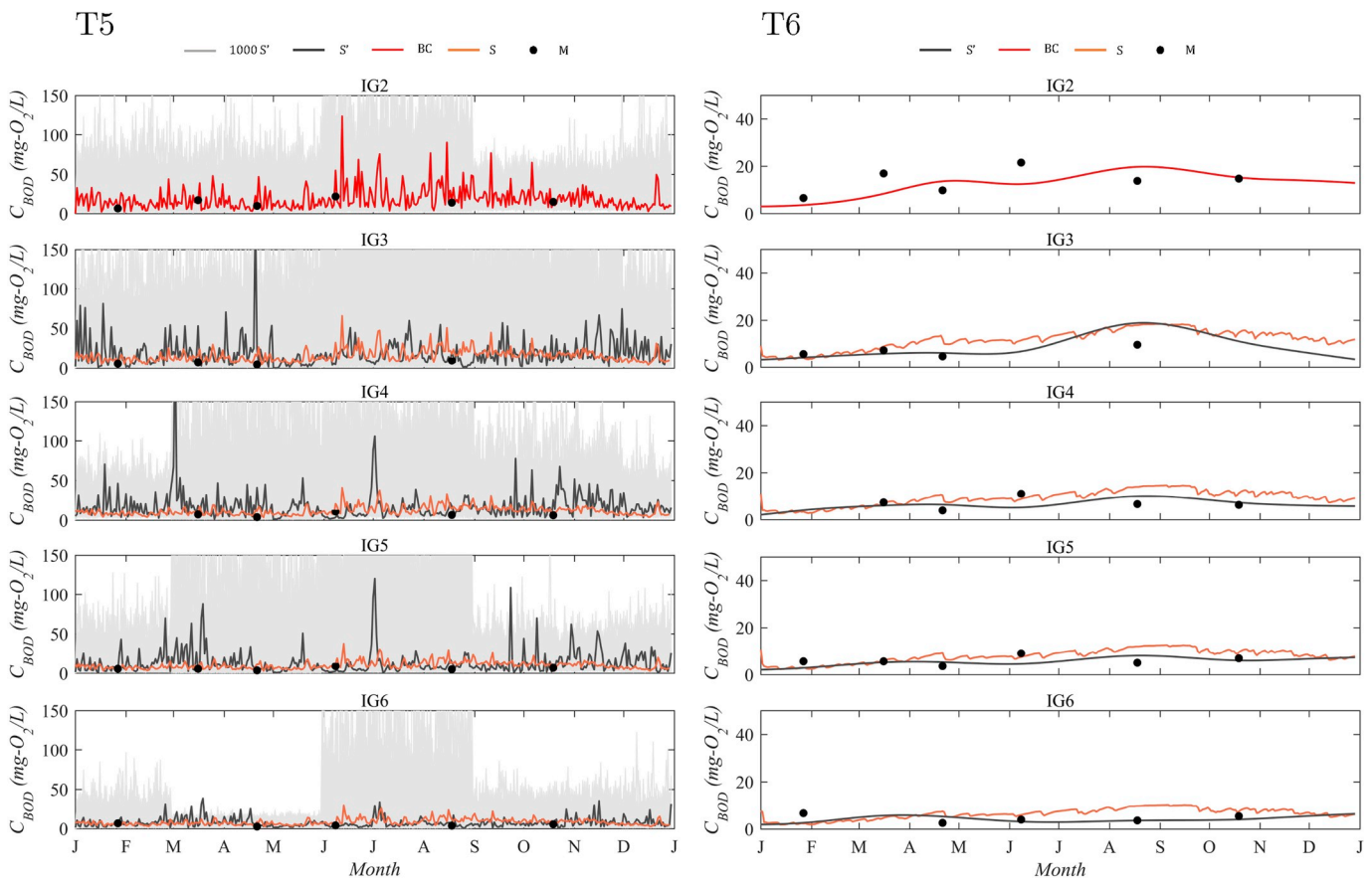

Fig. 5. Simulated daily concentrations (S) with boundary condition (BC) generated by test T5 and T6, monitoring data (M) of 2010 in each section and synthetic series (*S'*).

for section IG2.

In general, boxplots of simulated data generated with test T2 and T6 as boundary condition have a smaller interquartile range for all sections (IG2 to IG6; boxplots *S*). Boxplots for T3, T4 and T5 are very similar for both synthetic and deterministic modelling; these three tests use the logarithm of concentrations as input, which may explain the similarity between results.

Figs. 4 and 5 (daily values predicted with T3 to T5) show that most concentrations peaks are generated during winter season (june to august). This possibly occurred because this period has the highest means and standard deviations of the monitored dataset – supported by the data presented in the supplementary material.

3.2. Water quality duration curves

This section presents the water quality duration curves for each test discussed in section 4.1, as displayed in Fig. 6. In addition, curves of modelling outputs under steady state and monitoring data (2005–2016) are presented.

This strategy combines the characteristics of a stream throughout the range of variability, without regarding the sequence of occurrence; it allows to guarantee flexibility for framework classifications, verify the frequency of transgressions, or to estimate critical periods and locations, defining adequate planning for water withdrawals, effluent releases and water use charges throughout the year.

In general, the results show an agreement between methodologies for concentrations with higher frequency occurrence. Representation of critical events, on the other hand, are divergent. The most accurate tests for synthetic pollutographs at IG2 are T1, T3, T4 and T5, as previously suggested in section 4.1.

Fig. 7 compares medians and concentrations with 10% ($C_{10\%}$) and 90% ($C_{90\%}$) of occurrence of SIHQUAL outputs with each boundary condition. Concentrations of steady modelling and monitoring data are also presented for reference. Results reveal the overall effects when choosing different upstream boundary conditions for the unsteady approach, in comparison with the historical dataset.

For all sections, most tests overestimated $C_{90\%}$ and underestimate $C_{10\%}$. In Table 2, that presents the difference between concentrations simulated with each test and monitored data in terms of medians, $C_{10\%}$ and $C_{90\%}$, it is shown that the overestimation for $C_{90\%}$ simulated with SIHQUAL ranges between 0.05 mg-O_2/L (IG5, T6) and 6.51 mg-O_2/L (IG3, T2).

For predicted $C_{10\%}$, absolute differences are between 3.95 (IG6, T1) and 39.42 mg-O_2/L (IG4, T6). Prediction of extreme events in this case are more sensible. Differences of simulated medians, on the other hand, ranged from 0.05 (IG6, T3) to 5.00 mg-O_2/L (IG3, T3).

4. Discussion

Experiments with synthetic series show that historical monitoring datasets are undoubtedly valuable, and the relationship between statistical measures should be considered when designing sampling strategies. In fact, expressions to estimate the number of samples required often use as reference medians and standard deviations (e. g. Williams et al., 2014).

Large concentration peaks are observed in the synthetic series, following expected seasonal fluctuation and indicating that these series are representing potential conditions not predicted by the conservation laws approach; in this case, the conditions are extreme events (high concentrations) due to low streamflow observed for this period, in which dilution effects are minimized. In a similar analysis, Siqueira et al. (2017) applied a deterministic hydrological model and an

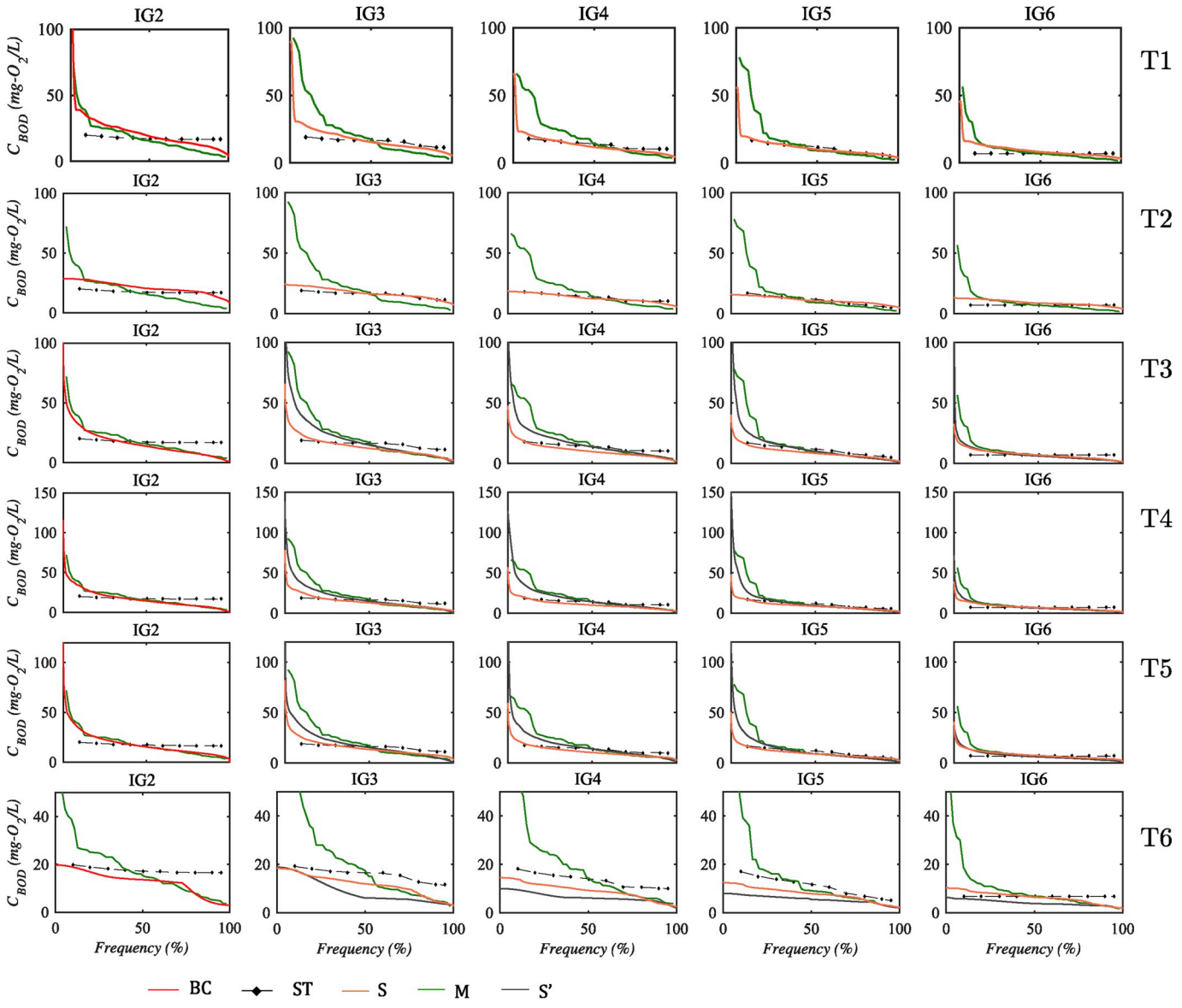

Fig. 6. Duration curves of historical monitoring dataset 2005–2016 (M) and simulations for 2010 with synthetic series (S′) and SIHQUAL results under unsteady (S) and steady (ST) state: tests T1 to T6 presented in each row.

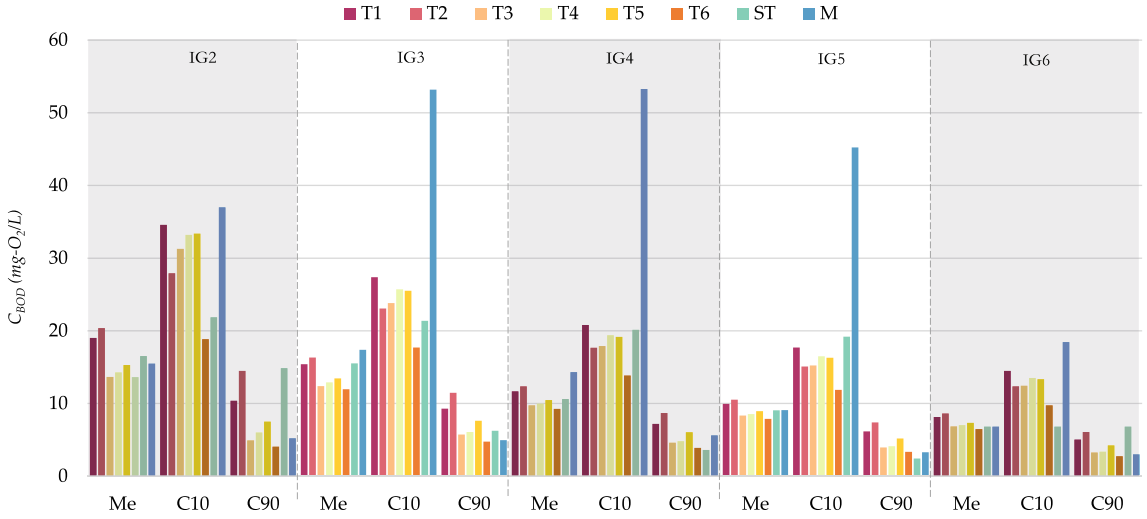

Fig. 7. Medians (Me), $C_{10\%}$ (C10) and $C_{90\%}$ (C90) of each simulated and monitored concentrations set.

Table 2
Difference of medians, $C_{10\%}$ and $C_{90\%}$ between monitored data and simulation results for each test ($C_{simulated} - C_{monitored}$; mg-$O_2$/L).

		T1	T2	T3	T4	T5	T6
IG2	Median	3.52	4.87	−1.83	−1.22	−0.19	−1.87
	$C_{10\%}$	−2.40	−9.08	−5.73	−3.79	−3.61	−18.15
	$C_{90\%}$	5.18	9.27	−0.28	0.82	2.32	−1.14
IG3	Median	−2.00	−1.06	−5.00	−4.50	−3.95	−5.43
	$C_{10\%}$	−25.81	−30.14	−29.39	−27.48	−27.68	−35.50
	$C_{90\%}$	4.35	6.51	0.79	1.12	2.68	−0.20
IG4	Median	−2.63	−1.95	−4.58	−4.32	−3.84	−5.05
	$C_{10\%}$	−32.48	−35.59	−35.38	−33.89	−34.11	−39.42
	$C_{90\%}$	1.57	3.07	−1.01	−0.82	0.42	−1.74
IG5	Median	0.87	1.45	−0.74	−0.53	−0.13	−1.21
	$C_{10\%}$	−27.52	−30.14	−30.01	−28.73	−28.93	−33.36
	$C_{90\%}$	2.86	4.11	0.67	0.82	1.88	0.05
IG6	Median	1.33	1.81	0.05	0.21	0.53	−0.33
	$C_{10\%}$	−3.95	−6.08	−5.99	−4.94	−5.10	−8.70
	$C_{90\%}$	2.05	3.07	0.25	0.38	1.26	−0.24

ensemble approach for flood forecasting. The latter technique provides a set of different scenarios for predicted discharges. The authors identified that, in comparison with the first forecast method, the ensemble ones showed higher accuracy and probability of detection for reference thresholds. Therefore, it is suggested that peaks may be better identified and predicted when different possible solutions are evaluated.

Results also indicate that, due to variation in the duration curves, upstream boundary may be responsible for uncertainty in simulation results; therefore, compromise decisions for strategies in water resources planning and management. Often used as calibration reference, for example, (e. g. Alaghmand et al., 2011; Wöhling et al., 2013), median outputs may also depend on the input pollutograph.

Several limitations of this study are acknowledged, emphasizing the need for additional future work: (i) analysis have been limited to one water quality constituent in a specific watershed; model performance may vary for different parameters and basin dynamics; (ii) the techniques applied to generate the synthetic pollutographs, although providing a valid method to compare model performance, are simplified; water quality time series are result of complex interactions in the environment; consequently, other methodologies to represent these interactions should also be evaluated; (iii) this study examined only one sampling strategy that represents common monitoring practice; strategies with different sampling frequencies (e.g., weekly or monthly), record lengths (e.g., 10 years), or approaches based on flow regime or storm observations are recommended in future studies; (iv) further calibration efforts accounting uncertainties in boundary conditions are also encouraged, since this approach might provide different parameter estimates and more robust predictions.

5. Conclusions

For water resources planning and management strategies, the concept of mathematical modelling allows integration of quantity (flow) and quality (concentrations). Input data, however, is a fundamental aspect to interpret results in this type of study. This research provides new contributions aiming to decrease the risk of inadequate decisions in water resources planning and management based on numerical simulations, integrating synthetic pollutographs and deterministic modelling. The proposed methodology aims to support more reliable analysis with available resources, considering that gather appropriate information at minimum cost remains a challenge (Hankin et al., 2016).

A few techniques to predict time series of BOD concentrations at regular time steps for a continuous period are evaluated. Empirical techniques are useful because they combine the many factors responsible for uncertainty in time series (missing data, non-linearity, seasonal and cyclical patterns etc), and demand a minimum description of cause and effect; the historical monitoring dataset provides the required knowledge about the system. The posterior phase, that propagates the information through deterministic equations, incorporates the different processes controlling release, transport and fate of pollutants in rivers. Consequently, strategies for water resources planning and management can be evaluated.

Interpolation with PCHIP function and Fourier series, although accounting for flow conditions effects on water quality, are sensitive to extreme values, since illogical concentrations were obtained in most river sections. Interpolation with smoothing spline had a gradual variation over time, not being able to represent the unsteady behavior.

The experiments with AR(1) processes demonstrated that preservation of seasonal mean and standard deviation possibly is an effective criterion to provide reasonable estimates of water quality.

Results suggest several important messages. Although not usually explored in deterministic water quality modelling under unsteady state, boundary conditions may have an important role in model outputs (even in concentrations of high frequency occurrence), and therefore impact calibration. Even though the tests performed in this study are simplified, they provide fast and parsimonious estimation of plausible different scenarios, and allow a conceptual analysis.

Although further calibration is required, SIHQUAL shows a systematic and consistent behavior in comparison with a natural system, being able to integrate and represent multiple scenarios of flow, input conditions and data availability. In such a context, this research provides background to evaluate the risk of disagreement with quality standards, complementing the information granted by monitoring programs and steady assessment.

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Appendix A. Supplementary data

Supplementary data to this article can be found online at https://doi.org/10.1016/j.jenvman.2019.03.047.

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